Release notes for ENDF/B Development n-011_Na_023 evaluation

April 26, 2017

- `psyche` Warnings:

  1. Strength function in URR not in agreement with PSYCHE's expectations
     FILE 2 / SECTION 151 / ISOTOPE MASS = 23. L = 0 / STRENGTH FUNCTION IS 1.04956E-05 / STRENGTH FUNCTION 1.04956E-05 / LIES OUTSIDE LIMITS 1.00000E-04 TO 9.00000E-04 (0): URR str. ftn.

```
FILE  2
   SECTION 151
        ISOTOPE MASS =  23. L =  0
                 STRENGTH FUNCTION IS  1.04956E-05
                                  STRENGTH FUNCTION 1.04956E-05
... [1 more lines]
```

  2. Gamma width not in agreement with PSYCHE's expectations
     FILE 2 / SECTION 151 / ISOTOPE MASS = 23. L = 1 / AT RESONANCE ENERGY 7.61700E+03 EV. THE GAMMA WIDTH 6.00000E-01 DEVIATES TOO MUCH FROM THE AVERAGE 3.58250E+00 (0): Gamma width

```
FILE  2
   SECTION 151
        ISOTOPE MASS =  23. L =  1
                 AT RESONANCE ENERGY  7.61700E+03 EV. THE GAMMA WIDTH  6.00000E-01 DEVIATES TOO MUCH FROM THE AV
```

  3. Gamma width not in agreement with PSYCHE's expectations
     FILE 2 / SECTION 151 / ISOTOPE MASS = 23. L = 1 / AT RESONANCE ENERGY 5.32200E+04 EV. THE GAMMA WIDTH 7.85000E-01 DEVIATES TOO MUCH FROM THE AVERAGE 3.58250E+00 (0): Gamma width

```
FILE  2
   SECTION 151
        ISOTOPE MASS =  23. L =  1
                 AT RESONANCE ENERGY  5.32200E+04 EV. THE GAMMA WIDTH  7.85000E-01 DEVIATES TOO MUCH FROM THE AV
```

  4. Gamma width not in agreement with PSYCHE's expectations
     FILE 2 / SECTION 151 / ISOTOPE MASS = 23. L = 2 / AT RESONANCE ENERGY 2.36710E+05 EV. THE GAMMA WIDTH 1.59000E+00 DEVIATES TOO MUCH FROM THE AVERAGE 5.88000E+00 (0): Gamma width

```
FILE  2
   SECTION 151
        ISOTOPE MASS =  23. L =  2
                 AT RESONANCE ENERGY  2.36710E+05 EV. THE GAMMA WIDTH  1.59000E+00 DEVIATES TOO MUCH FROM THE AV
```

- `linear` Errors:

  1. Negative cross section found
     0: Neg. Sig(E)

```
 Linearize ENDF/B Cross Sections (LINEAR 2015-1)
 ------------------------------------------------------------------------------
 Retrieval Criteria-----------        MAT
 Monitor Mode-----------------        Off
 Minimum Cross Section-------- 1.0000E-10 (Default Option)
... [72 more lines]
```

- `recent` Warnings:

  1. Competative widths aren't all zero like they're supposed to be
     0: LRX=0

```
Calculate Cross Sections from Resonance Parameters (RECENT 2015-1)
===============================================================================
Retrieval Criteria----------        MAT
File 2 Mimimum Cross Section- 1.0000E-10 (Standard Option)
Reactions with No Background-     Output (Resonance Contribution)
... [222 more lines]
```

- `fudge-4.0` Warnings:

  1. Missing a channel with a particular angular momenta combination
     resonances / resolved (Error # 1): missingResonanceChannel

```
WARNING: Missing a channel with angular momenta combination L = 0, J = 0.0 and S = 0.0 for "capture"
WARNING: Missing a channel with angular momenta combination L = 1, J = 1.0 and S = 0.0 for "capture"
WARNING: Missing a channel with angular momenta combination L = 1, J = 1.0 and S = 1.0 for "capture"
WARNING: Missing a channel with angular momenta combination L = 1, J = 2.0 and S = 1.0 for "capture"
        ... plus 6 more instances of this message
```

  2. For distributions, flat interpolation along incident energy is unphysical!
     production label 24: /reactionSuite/reactions/production[@label='24'] / Product: gamma / Distribution: / uncorrelated - energy - XYs2d: (Error # 0): flatIncidentEnergyInterpolation

```
WARNING: For distributions, flat interpolation along incident energy is unphysical!
```

  3. Cross section does not match sum of linked reaction cross sections
     crossSectionSum label 0: total (Error # 0): CS Sum.

```
WARNING: Cross section does not match sum of linked reaction cross sections! Max diff: 12.07%
```

  4. Cross section does not match sum of linked reaction cross sections
     crossSectionSum label 1: nonelastic (Error # 0): CS Sum.

```
WARNING: Cross section does not match sum of linked reaction cross sections! Max diff: 1.17%
```

  5. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
     Section 1 (n + Na23): / Form 'eval': / Component 1 (Error # 0): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (0.000000e+00) is too small
```

  6. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
     Section 2 ((z,n)): / Form 'eval': (Error # 0): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (0.000000e+00) is too small
```

  7. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
     Section 3 (n[multiplicity:'2'] + Na22): / Form 'eval': / Component 0 (Error # 0): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (0.000000e+00) is too small
```

8. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
Section 3 (n[multiplicity:'2'] + Na22): / Form 'eval': / Component 1 (Error # 0): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (0.000000e+00) is too small
```

9. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
Section 4 (Na24 + gamma): / Form 'eval': (Error # 0): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (4.246430e-11) is too small
```

10. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
Section 5 (H1 + Ne23_s): / Form 'eval': (Error # 0): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (0.000000e+00) is too small
```

11. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
Section 6 (He4 + F20_s): / Form 'eval': (Error # 0): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (0.000000e+00) is too small
```

12. The ratio of smallest/largest eigenvalue is quite small, possibly leading to numerical instability in downstream codes.
Section 7 (n + Na23 [angular distribution]): / Form 'eval': (Error # 1): Condition num.

```
WARNING: Ratio of smallest/largest eigenvalue (0.000000e+00) is too small
```

- `fudge-4.0` Errors:

1. The spin statistical weights are off, indicating missing channels
resonances / resolved / MultiLevel_BreitWigner (Error # 0): badSpinStatisticalWeights

```
WARNING: The spin statical weights for L=1 sums to 2.0, but should sum to 3.0.  You have too few channels for re
WARNING: The spin statical weights for L=2 sums to 1.875, but should sum to 5.0.  You have too few channels for
```

2. Calculated and tabulated Q values disagree.
reaction label 20: n[multiplicity:'2'] + Na22 (Error # 0): Q mismatch

```
WARNING: Calculated and tabulated Q-values disagree: -12678175.35817719 eV vs -1.2414e7 eV!
```

3. Calculated and tabulated Q values disagree.
reaction label 21: Na24 + gamma (Error # 0): Q mismatch

```
WARNING: Calculated and tabulated Q-values disagree: 6700137.276607513 eV vs 6959490. eV!
```

4. Calculated and tabulated Q values disagree.
reaction label 22: H1 + Ne23_s (Error # 0): Q mismatch

```
WARNING: Calculated and tabulated Q-values disagree: -3852902.2970047 eV vs -3.597e6 eV!
```

5. Calculated and tabulated Q values disagree.
   reaction label 23: He4 + F20_s (Error # 0): Q mismatch

```
WARNING: Calculated and tabulated Q-values disagree: -4125488.268978119 eV vs -3.866e6 eV!
```

6. A covariance matrix was not positive semi-definite, so it has negative eigenvalues.
   Section 7 (n + Na23 [angular distribution]): / Form 'eval': / LegendreLValue L=1 vs 1 (Error # 0): Bad evs

```
WARNING: 6 negative eigenvalues! Worst case = -2.321350e-06
```

- `njoy2012` Warnings:

1. Evaluation has no unresolved resonance parameters given
   unresr...calculation of unresolved resonance cross sections (0): No URR

```
 ---message from unresr---mat 1125 has no unresolved parameters
                          copy as is to nout
```

2. Evaluation has no unresolved resonance parameters given
   purr...probabalistic unresolved calculation (0): No URR

```
 ---message from purr---mat 1125 has no unresolved parameters
                          copy as is to nout
```

3. With the advent of the ENDF-6 format, it is possible to make evaluations that fully describe all the products of a nuclear reaction. Some carry-over evaluations from earlier ENDF/B versions also have this capability, but many do not. This message is intended to goad evaluators to improve things!
   groupr...compute self-shielded group-averaged cross-sections (0): GROUPR/conver (0)

```
 ---message from conver---cannot do complete particle production for mt= 16
                          only mf4/mf5 provided
```

4. With the advent of the ENDF-6 format, it is possible to make evaluations that fully describe all the products of a nuclear reaction. Some carry-over evaluations from earlier ENDF/B versions also have this capability, but many do not. This message is intended to goad evaluators to improve things!
   groupr...compute self-shielded group-averaged cross-sections (1): GROUPR/conver (0)

```
 ---message from conver---cannot do complete particle production for mt= 91
                          only mf4/mf5 provided
```

5. Only partial urr covariance data was given.
   errorr...produce cross section covariances (0): ERRORR/resprx (5)

```
 ---message from resprx---mf2 nls=3, but mf32 nls=0
                          continue with partial urr covariance data
```

6. No scattering radius uncertainty given.
   errorr...produce cross section covariances (1): ERRORR/rpxlc12 (0)

```
 ---message from rpxlc12---no scattering radius uncertainty
```

7. Generic warning message
   errorr...produce cross section covariances (2): Warning

```
 ---message from rpxlc12---resonance parameter loop done                 9.4s
```

8. Generic warning message
   errorr...produce cross section covariances (3): Warning

```
 ---message from rpxlc12---sensitivity calculation continues             9.5s
```

9. Generic warning message
   errorr...produce cross section covariances (4): Warning

```
 ---message from rpxlc12---sensitivity calculation completed             9.7s
```

- `acelst` Warnings:

1. generic warning message
   0: Warning

```
 ACELST WARNING - More than one range for MF/MT          6          91
STOP ACELST Completed
```

- `endf2htm` Warnings:

1. Build of a section of the HTML page failed because the format hasn't been implemented in ENDF2HTM.
   MF32MT151: Unimplemented

```
At line 2659 of file endf.f
Fortran runtime error: Bad value during integer read
```